Alizarin

72-48-0 | DTXSID5045960

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 40.4 days

Global applicability domain: Outside

Local applicability domain index: 2.60e-01

Confidence level: 8.09e-01

Nearest Neighbors from the Training Set

Image not found
9-Ethyl-9H-fluorene
Measured: 2330
Predicted: N/A

Image not found
2-Methylphenanthrene
Measured: 1370
Predicted: 25.0

Image not found
Phenanthrene, trimethyl-
Measured: 26200
Predicted: 75.6

Image not found
1-Methyl phenanthrene
Measured: 1370
Predicted: 36.9

Image not found
1-Methylpyrene
Measured: 33300
Predicted: 94.4